Calculation of Second Topological Moment $\langle m^2 \rangle$ of Two Entangled Polymers

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We set up a Chern-Simons theory for the entanglement of two polymers P_1 and P_2, and calculate the second topological moment $\langle m^2 \rangle$, where m is the linking number. The result approximately to a polymer in an ensemble of many others, which are considered as a single very long effective polymer.

I. THE PROBLEM

Consider two polymers P_1 and P_2 which statistically can be linked with each other any number of times $m = 0, 1, 2, \ldots$. The situation is illustrated in Fig. 1 for $m = 2$.

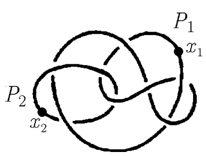

FIG. 1. Closed polymers P_1, P_2 with trajectories C_1, C_2 respectively.

We would like to find the probability distribution of the linking numbers m as a function of the lengths of P_1 and P_2. As a first contribution to solving this problem we calculate, in this note, the second moment of this distribution, $\langle m^2 \rangle$. The self-entanglements are ignored.

The solution of this two-polymer problem may be considered as an approximation to a more interesting physical problem in which a particular polymer is linked to any number N of polymers, which are effectively replaced by a single long "effective" polymer [1].

Let $G_m(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2)$ be the configurational probability to find the polymer P_1 of length L_1 with fixed coinciding end points at $\mathbf{x}_1$ and the polymer P_2 of length L_2 with fixed coinciding end points at $\mathbf{x}_2$, entangled with a Gaussian linking number m.

The second moment $\langle m^2 \rangle$ is defined by the ratio of integrals

$$\langle m^2 \rangle = \frac{\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \int_{-\infty}^{+\infty} dm\; m^2 G_m(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2)}{\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \int_{-\infty}^{+\infty} dm\, G_m(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2)} \quad (1)$$

performed for either of the two probabilities. The integrations in $d^3\mathbf{x}_1 d^3\mathbf{x}_2$ covers all positions of the end points. The denominator plays the role of a partition function of the system:

$$Z \equiv \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \int_{-\infty}^{+\infty} dm\, G_m(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2) \quad (2)$$

Due to the translational invariance of the system, the probabilities depend only on the differences between the end point coordinates:

$$G_m(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2) = G_m(\mathbf{x}_1 - \mathbf{x}_2; L_1, L_2) \quad (3)$$

Thus, after the shift of variables, the spatial double integrals in (1) can be rewritten as

$$\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 G_m(\mathbf{x}_1 - \mathbf{x}_2; L_1, L_2) = V \int d^3\mathbf{x} G_m(\mathbf{x}; L_1, L_2), \quad (4)$$

where V denotes the total volume of the system.

II. POLYMER FIELD THEORY FOR PROBABILITIES

The linking number for the two polymers is given by the Gauss integral

$$I_G(P_1, P_2) = \frac{1}{4\pi} \oint_{P_1} \oint_{P_2} [d\mathbf{x}_1 \times d\mathbf{x}_2] \cdot \frac{\mathbf{x}_1 - \mathbf{x}_2}{|\mathbf{x}_1 - \mathbf{x}_2|^3}. \quad (5)$$

It takes the values $m = 0, \pm 1, \pm 2, \ldots$. With the help of two vector potentials $\mathbf{A}_1$ and $\mathbf{A}_2$, the phase factor $e^{im\lambda}$ can be obtained as a result of a local gauge theory of the Chern-Simons type:

$$e^{im\lambda} = \int \mathcal{D}A_1^\mu \mathcal{D}A_2^\mu \times e^{-\mathcal{A}_{\mathrm{CS}} - \kappa \int_{P_1} d\mathbf{x}_1 \cdot \mathbf{A}_1 - \lambda \int_{P_2} d\mathbf{x}_2 \cdot \mathbf{A}_2}, \quad (6)$$

where $\mathcal{A}_{\mathrm{CS}}$ is the action

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$$\mathcal{A}_{\rm CS} = i\kappa \int d^3\mathbf{x}\, \varepsilon_{\mu\nu\rho} A_1^\mu \partial_\nu A_2^\rho, \tag{7}$$

Indeed, the correlation functions $D_{ij}^{\mu\nu}(\mathbf{x},\mathbf{x}')$ of the gauge fields are

$$\langle A_1^\mu(\mathbf{x}) A_1^\nu(\mathbf{x}')\rangle = 0, \quad \langle A_2^\mu(\mathbf{x}) A_2^\nu(\mathbf{x}')\rangle = 0, \tag{8}$$

$$\langle A_1^\mu(\mathbf{x}) A_2^\nu(\mathbf{x}')\rangle = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \frac{i\epsilon_{\mu\lambda\nu} k^\lambda}{\mathbf{k}^2} \tag{9}$$

$$= \frac{1}{4\pi} \epsilon_{\mu\lambda\nu} \nabla_\lambda \frac{1}{|\mathbf{x}-\mathbf{x}'|}$$

$$= \frac{1}{4\pi} \epsilon_{\mu\nu\kappa} \frac{(x-x')^\lambda}{|\mathbf{x}-\mathbf{x}'|^3}, \tag{10}$$

such that the functional integral on the right-hand side of (6) produces directly the phase factor $e^{iI_G(P_1,P_2)\lambda}$ with the eigenvalue $e^{im\lambda}$.

We can select configurations with a certain linking number m from all configurations by forming the integral $\int_{-\infty}^{\infty} d\lambda e^{-im\lambda}$ over this quantity.

The most efficient way of describing the statistical fluctuations of the polymers P_1 and P_2 is by two complex polymer fields $\psi_1^{a_1}(\mathbf{x}_1)$ and $\psi_2^{a_2}(\mathbf{x}_2)$ with n_1 and n_2 replica ($a_1 = 1,\ldots,n_1,\ a_2 = 1,\ldots,n_2$). At the end we shall take $n_1, n_2 \to 0$ to ensure that these fields describe only one polymer each [2]. For these fields we define an auxiliary probability $G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z})$ to find the polymer P_1 with open ends at $\mathbf{x}_1, \mathbf{x}_1'$ and the polymer P_2 with open ends at $\mathbf{x}_2, \mathbf{x}_2'$. The double vectors $\vec{\mathbf{x}}_1 \equiv (\mathbf{x}_1, \mathbf{x}_1')$ and $\vec{\mathbf{x}}_2 \equiv (\mathbf{x}_2, \mathbf{x}_2')$ collect initial and final endpoints of the two polymers P_1 and P_2. The auxiliary probability $G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z})$ is given by a functional integral

$$G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}) = \lim_{n_1,n_2\to 0} \int \mathcal{D}(\text{fields})$$
$$\times \psi_1^{a_1}(\mathbf{x}_1) \psi_1^{*a_1}(\mathbf{x}_1') \psi_2^{a_2}(\mathbf{x}_2) \psi_2^{*a_2}(\mathbf{x}_2') e^{-\mathcal{A}} \tag{11}$$

where $\mathcal{D}(\text{fields})$ indicates the measure of functional integration, and $\mathcal{A}$ the action governing the fluctuations. It consists of kinetic terms for the fields, a quartic interaction of the fields to account for the fact that two monomers of the polymers cannot occupy the same point, the so-called *excluded-volume effect*, and a Chern-Simons field to describe the linking number m. Neglecting at first the excluded-volume effect and focusing attention on the linking problem only, the action reads

$$\mathcal{A} = \mathcal{A}_{\rm CS} + \mathcal{A}_{\rm pol}, \tag{12}$$

with a polymer field action

$$\mathcal{A}_{\rm pol} = \sum_{i=1}^{2} \int d^3\mathbf{x} \left[|\bar{\mathbf{D}}^i \Psi_i|^2 + m_i^2 |\Psi_i|^2 \right]. \tag{13}$$

in which we have omitted a gauge fixing term, which enforces the Lorentz gauge. They are coupled to the polymer fields by the covariant derivatives

$$\mathbf{D}^i = \boldsymbol{\nabla} + i\gamma_i \mathbf{A}^i, \tag{14}$$

with the coupling constants $\gamma_{1,2}$ given by

$$\gamma_1 = \kappa \qquad \gamma_2 = \lambda. \tag{15}$$

The square masses of the polymer fields contain the chemical potentials $z_{1,2}$ of the polymers:

$$m_i^2 = 2Mz_i. \tag{16}$$

They are conjugate variables to the length parameters L_1 and L_2, respectively. The symbols Ψ_i collect the replica of the two polymer fields

$$\Psi_i = \left(\psi_i^1, \ldots, \psi_i^{n_i}\right), \quad \Psi_i^* = \left(\psi_i^{*1}, \ldots, \psi_i^{*n_i}\right), \tag{17}$$

and their absolute squares contain the sums over the replica

$$|\mathbf{D}^i \bar{\Psi}_i|^2 = \sum_{a_i=1}^{n_i} |\mathbf{D}^i \psi_i^{a_i}|^2, \quad |\Psi_i|^2 = \sum_{a_i=1}^{n_i} |\psi_i^{a_i}|^2. \tag{18}$$

Having specified the fields, we can now write down the measure of functional integration in Eq. (11):

$$\mathcal{D}(\text{fields}) = \int \mathcal{D}A_1^\mu \mathcal{D}A_2^\mu \mathcal{D}\Psi_1 \mathcal{D}\Psi_1^* \mathcal{D}\Psi_2 \mathcal{D}\Psi_2^*. \tag{19}$$

By Eq. (6), the parameter λ is conjugate to the linking number m. We can therefore calculate the desired probability $G_m(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; L_1, L_2)$ from the auxiliary one $G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z})$ by the following Laplace integrals $\vec{z} = (z_1, z_1)$:

$$G_m(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; L_1, L_2) = \lim_{\substack{\mathbf{x}_1'\to\mathbf{x}_1 \\ \mathbf{x}_2'\to\mathbf{x}_2}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i} \frac{dz_2}{2\pi i} e^{(z_1L_1+z_2L_2)}$$
$$\times \int_{-\infty}^{\infty} d\lambda e^{-im\lambda} G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}). \tag{20}$$

III. CALCULATING THE PARTITION FUNCTION

Let us use the polymer field theory to calculate the partition function (2). By Eq. (20), it is given by the integral over the auxiliary probabilities

$$Z = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{\mathbf{x}_1'\to\mathbf{x}_1 \\ \mathbf{x}_2'\to\mathbf{x}_2}} \int_{c-i\infty}^{c+\infty} \frac{dz_1}{2\pi i} \frac{dz_2}{2\pi i} e^{(z_1L_1+z_2L_2)}$$
$$\times \int_{-\infty}^{+\infty} dm \int_{-\infty}^{+\infty} d\lambda e^{-im\lambda} G_\lambda(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}). \tag{21}$$

The integration over dm is trivial and gives $2\pi\delta(\lambda)$, enforcing $\lambda = 0$, so that

$$Z = -\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{\mathbf{x}_1\to\mathbf{x}_1 \\ \mathbf{x}'_2\to\mathbf{x}_2}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1 dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)} \times \; G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right) \tag{22}$$

To compute $G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)$ we observe that the action $\mathcal{A}$ in Eq. (12) is quadratic in λ. Let us expand $\mathcal{A}$ as

$$\mathcal{A} = \mathcal{A}_0 + \lambda\mathcal{A}_1 + \lambda^2\mathcal{A}_2 \tag{23}$$

where

$$\mathcal{A}_0 \equiv \mathcal{A}_{\text{CS}} + \int d^3\mathbf{x}\left[|\mathbf{D}_1\Psi_1|^2 + |\boldsymbol{\nabla}\Psi_2|^2 + \sum_{i=1}^{2}|\Psi_i|^2\right], \tag{24}$$

a linear coefficient

$$\mathcal{A}_1 \equiv \int d^3\mathbf{x}\; \mathbf{j}_2(\mathbf{x})\cdot\mathbf{A}_2(\mathbf{x}) \tag{25}$$

with a "current" of the second polymer field

$$\mathbf{j}_2(\mathbf{x}) = i\Psi_2^*(\mathbf{x})\boldsymbol{\nabla}\Psi_2(\mathbf{x}), \tag{26}$$

and a quadratic coefficient

$$\mathcal{A}_2 \equiv \frac{1}{4}\int d^3\mathbf{x}\; \mathbf{A}_2^2|\Psi_2(\mathbf{x})|^2. \tag{27}$$

With these definitions we can rewrite (23) as

$$G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right) = \int \mathcal{D}(\text{fields})e^{-\mathcal{A}_0} \times\psi_1^{a_1}(\mathbf{x}_1)\psi_1^{*a_1}(\mathbf{x}'_1)\psi_2^{a_2}(\mathbf{x}_2)\psi_2^{a_2}(\mathbf{x}') \tag{28}$$

From Eq. (24) it is clear that $G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)$ is the product of the configurational probabilites of two free polymers.

Note that the fields Ψ_2, Ψ_2^* are free, whereas the fields Ψ_1, Ψ_1^* are apparently not free because of the couplings with the Chern-Simons fields through the covariant derivative $\mathbf{D}^1$. This is, however, an illusion: the fields A_μ^i have a vanishing diagonal propagators $\langle A_\mu^i A_\nu^i\rangle = 0$. integrating out A_2^μ in (28), we find the flatness condition:

$$\varepsilon^{\mu\nu\rho}\partial_\nu A_\mu^i = 0. \tag{29}$$

On a flat space with vanishing boundary conditions at infinity this implies $A_1^\mu = 0$. As a consequence, the functional integral (28) factorizes

$$G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right) = G_0(\mathbf{x}_1 - \mathbf{x}'_1; z_1)G_0(\mathbf{x}_2 - \mathbf{x}'_2; z_2), \tag{30}$$

where $G_0(\mathbf{x}_i - \mathbf{x}'_i; z_i)$ are the free correlation functions of the polymer fields:

$$G_0(\mathbf{x}_i - \mathbf{x}'_i; z_i) = \langle\psi_i^{a_i}(\mathbf{x}_i)\psi_i^{*a_i}(\mathbf{x}'_i)\rangle. \tag{31}$$

In momentum space, the correlation functions are

$$\langle\tilde{\psi}^{a_i}(\mathbf{k}_i)\tilde{\psi}_i^{*a_i}(\mathbf{k}'_i)\rangle = \delta^{(3)}\left(\mathbf{k}_i + \mathbf{k}'_i\right)\frac{1}{\mathbf{k}_i^2 + m_i^2} \tag{32}$$

such that

$$G_0(\mathbf{x}_i - \mathbf{x}'_i; z_i) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}\frac{1}{\mathbf{k}_i^2 + m_i^2}, \tag{33}$$

and

$$G_0(\mathbf{x}_i - \mathbf{x}'_i; L_i) = \int_{c-i\infty}^{c+i\infty}\frac{dz_i}{2\pi i}e^{z_i L_i}G_0(\mathbf{x}_i - \mathbf{x}'_i; z_i) = \frac{1}{4\sqrt{2}M}\left(\frac{M}{2\pi}\right)^{3/2} L_i^{-3/2}e^{-M(\mathbf{x}_i - \mathbf{x}'_i)/2L_i}. \tag{34}$$

Thus we obtain for (22):

$$Z = 2\pi\int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \times \lim_{\substack{\mathbf{x}'_1\to\mathbf{x}_1 \\ \mathbf{x}'_2\to\mathbf{x}_2}} G_0(\mathbf{x}_1 - \mathbf{x}'_1; L_1)G_0(\mathbf{x}_2 - \mathbf{x}'_2; L_2) \tag{35}$$

The integrals at coinciding end points can easily be performed, and we find

$$Z = \frac{2\pi M V^2}{(8\pi)^3}(L_1 L_2)^{-3/2} \tag{36}$$

It is important to realize that in Eq. (21), the limits of coinciding end points $\mathbf{x}'_i \to \mathbf{x}_i$ and the inverse Laplace transformations do not commute unless a proper renormalization scheme is chosen to eliminate the divergences caused by the insertion of the composite operators $|\psi(r)|^2$. This can be seen for a single polymer P. If we were to commuting the limit of coinciding end points with the Laplace transform, we would obtain

$$\int_{c-i\infty}^{c+i\infty}\frac{dz}{2\pi}e^{zL}\lim_{\mathbf{x}'\to\mathbf{x}}G_0(\mathbf{x} - \mathbf{x}'; z) = \int_{c-i\infty}^{c+i\infty}\frac{dz}{2\pi i}e^{zL}G_0(\mathbf{0}, z), \tag{37}$$

where

$$G_0(\mathbf{0}; z) = \langle|\psi(\mathbf{x})|^2\rangle. \tag{38}$$

This expectation value, however, is linearly divergent:

$$\langle|\psi(\mathbf{x}_a)|^2\rangle = \int\frac{d^3k}{k^2 + m^2} \to \infty \tag{39}$$

IV. CALCULATION OF NUMERATOR IN SECOND MOMENT

Let us now turn to the numerator in Eq. (1):

$$N \equiv \int d^2\mathbf{x}_1 d^3\mathbf{x}_2 \int_{-\infty}^{\infty} dm\ m^2 G_m\left(\mathbf{x}_1, \mathbf{x}_2; L_1, L_2\right). \quad (40)$$

We set up a functional integral for N in terms of the auxiliary probability $G_{\lambda=0}\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)$ analogous to Eq. (21):

$$N = \int d^3\mathbf{x}_1 d^3 r_2 \int_{-\infty}^{\infty} dm\ m^2 \lim_{\substack{\mathbf{x}_1' \to \mathbf{x} \\ \mathbf{x}' \to \mathbf{x}_2}} \int_{c-i\infty}^{c_\tau i\infty} \frac{dz_i}{2\pi i}\frac{dz_2}{2\pi i}$$
$$e^{(z_1 L_1 + z_2 L_2)} \int_{-\infty}^{\infty} d\lambda e^{-im\lambda} G_\lambda\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right). \quad (41)$$

The integration in dm is easily performed after noting that

$$\int_{-\infty}^{\infty} dm\ m^2 e^{-im\lambda} G_\lambda\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)$$
$$= -\int_{-\infty}^{\infty} dm \left(\frac{\partial^2}{\partial\lambda^2} e^{-im\lambda}\right) G_\lambda\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right). \quad (42)$$

After a double integration by parts in λ, and an integration in m, we obtain

$$N = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{\mathbf{x}_1' \to \mathbf{x}_1 \\ \mathbf{x}_2' \to \mathbf{x}_2}} (-1) \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)}$$
$$\int_{-\infty}^{\infty} d\lambda\ \delta(\lambda) \left[\frac{\partial^2}{\partial\lambda^2} G_\lambda\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)\right] \quad (43)$$

Performing the now trivial integration in $d\lambda$ yields

$$N = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{\mathbf{x}_1' \to \mathbf{x}_1 \\ \mathbf{x}_2' \to \mathbf{x}_2}} (-1) \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)}$$
$$\times \left[\frac{\partial^2}{\partial\lambda^2} G_\lambda\left(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2; \vec{z}\right)\right]_{\lambda=0} \quad (44)$$

To compute the term in brackets, we use again Eq. (23) and Eqs. (24) –(49), and find

$$N = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)}$$
$$\times \int \mathcal{D}(\text{fields})\ \exp(-\mathcal{A}_0) |\psi_1^{a_1}(\mathbf{x}_1)|^2 |\psi_2^{a_2}(\mathbf{x}_2)|^2$$
$$\times \left[\left(\int d^3\mathbf{x}\, \mathbf{A}_2 \cdot \Psi_2^* \boldsymbol{\nabla} \Psi_2\right)^2 + \frac{1}{2}\int d^3\mathbf{x}\, \mathbf{A}_2^2 \,|\Psi_2|^2\right]. \quad (45)$$

In this equation we have taken the limits of coinciding endpoint inside the Laplace integral over z_1, z_2. This will be justified later on the grounds that the potentially dangerous Feynman diagrams containing the insertions of operations like $|\Psi_i|^2$ vanish in the limit $n_1, n_2 \to 0$.

In order to calculate (45), we decompose the action into a free part

$$\mathcal{A}_0^0 \equiv \mathcal{A}_{\text{CS}}$$
$$+ \int d^3\mathbf{x} \left[|\mathbf{D}^1 \Psi_1|^2 + |\boldsymbol{\nabla}\Psi_2|^2 + \sum_{i=1}^{2} 2|\Psi_i|^2\right], \quad (46)$$

and interacting parts

$$\mathcal{A}_1^0 \equiv \int d^3\mathbf{x}\ \mathbf{j}_1(\mathbf{x}) \cdot \mathbf{A}_1(\mathbf{x}) \quad (47)$$

with a “current” of the first polymer field

$$\mathbf{j}_1(\mathbf{x}) \equiv i\Psi_1^*(\mathbf{x}) \boldsymbol{\nabla} \Psi_1(\mathbf{x}), \quad (48)$$

and

$$\mathcal{A}_0^2 \equiv \frac{1}{4}\int d^3\mathbf{x}\ \mathbf{A}_1^2 |\Psi_1(\mathbf{x})|^2. \quad (49)$$

Expanding the exponential

$$e^{\mathcal{A}_0} = e^{\mathcal{A}_0^0 + \mathcal{A}_0^1 + \mathcal{A}_0^2} = e^{\mathcal{A}_0}\left[1 - \mathcal{A}_0^1 + \frac{(\mathcal{A}_0^1)^2}{2} - \mathcal{A}_0^2 + \dots\right], \quad (50)$$

and keeping only the relevant terms, the functional integral (45) can be rewritten as a purely Gaussian expectation value

$$N = \kappa^2 \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)}$$
$$\times \int \mathcal{D}(\text{fields})\ \exp(-\mathcal{A}_0^0) |\psi_1^{a_1}(\mathbf{x}_1)|^2 |\psi_2^{a_2}(\mathbf{x}_2)|^2$$
$$\times \left[\left(\int d^3\mathbf{x}\, \mathbf{A}_1 \cdot \Psi_1^* \boldsymbol{\nabla} \Psi_1\right)^2 + \frac{1}{2}\int d^3\mathbf{x}\, \mathbf{A}_1^2 \,|\Psi_1|^2\right]$$
$$\times \left[\left(\int d^3\mathbf{x}\, \mathbf{A}_2 \cdot \Psi_2^* \boldsymbol{\nabla} \Psi_2\right)^2 + \frac{1}{2}\int d^3\mathbf{x}\, \mathbf{A}_2^2 \,|\Psi_2|^2\right] \quad (51)$$

Only four diagrams shown in Fig. (2) contribute in Eq. (51).

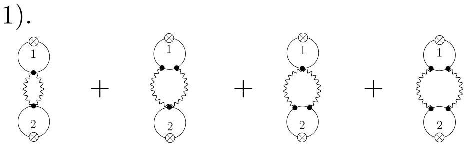

FIG. 2. Four diagrams contributing in Eq. (51). The lines indicate correlation functions of Ψ_i-fields. The crossed circles with label i denote the insertion of $|\Psi_i(\mathbf{x}_i)|^2$.

Note that the initially asymmetric treatment of polymers P_1 und P_2 in the action (12) has led to a completely symmetric expression for the second moment.

Only the first diagram in Fig. 2 is divergent due to the divergence of the loop formed by two vector correlation functions. This infinity may be absorbed in the four-Ψ interaction accounting for the excluded volume effect which we do not consider at the moment. No divergence arises from the insertiona of the composite fields $|\Psi_i(\mathbf{x}_i)|^2$. In this respect, the disconnected diagrams shown in Fig. 3 are potentially dangerous.

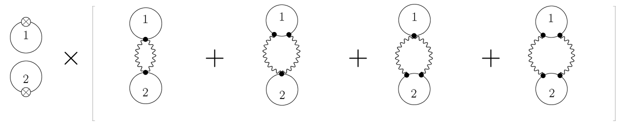

FIG. 3. Four diagrams contributing in Eq. (51). The lines indicate correlation functions of Ψ_i-fields. The crossed circles with label i denote the insertion of $|\Psi_i(\mathbf{x}_i)|^2$.

But these vanish in the limit of zero replica indices $n_1, n_2 \to 0$.

V. CALCULATION OF FIRST FEYNMAN DIAGRAMS IN FIG. 2

From Eq. (51) one has to evaluate the following integral

$$N_1 = \frac{\kappa^2}{4} \lim_{\substack{n_1\to 0\\ n_2\to 0}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1L_1+z_2L_2)} \int d^3x_1 d^3x_2 \int d^3x_1' d^3x_2' \left\langle |\psi_1^{a_1}(\mathbf{x}_1)|^2 |\psi_2^{a_2}(\mathbf{x}_2)|^2 \left(|\Psi_1|^2 \mathbf{A}_1^2\right)_{\mathbf{x}_1'} \left(|\Psi_2|^2 \mathbf{A}_2^2\right)_{\mathbf{x}_2'} \right\rangle. \tag{52}$$

There is an ultraviolet-divergent contribution which should be properly regularized. The system has, of course, a microscopic scale, which is the size of the momomers. This, however, is not the appropriate short-distance scale to be uses here. The model treats the polymers as random chains. However, the momomers of a polymer in the laboratory are usually not freely movable, so that polymers have a certain stiffness. This gives rise to a certain persistence length ξ_0 over which a polymer is stiff. This length scale is increased to $\xi > \xi_0$ by the excluded-volume effects. This is the length scale which should be used as a proper physical short-distance cutoff. We may impose this cutoff by imagining the model as being defined on a simple cubic lattice of spacing ξ. This would, of course, make analytical calculations quite difficult. Still, as we shall see, it is possible to estimate the dependence of the integral N_1 and the others in the physically relevant limit in which the lengths of the polymers are much larger than the persistence length ξ.

An alternative and simpler regularization is based on cutting off all ultraviolet-divergent continuum integrals at distances smaller than ξ.

After such a regularization, the calculation of N_1 is rather straightforward. Replacing the expectation values by the Wick contractions corresponding to the first diagram in Fig. 2, and performing the integrals as shown in the Appendix, we obtain

$$N_1 = \frac{V}{4\pi}\frac{M^2}{(8\pi)^6}(L_1L_2)^{-\frac{1}{2}} \times \int_0^1 ds\,[(1-s)s]^{-\frac{3}{2}} \int d^3x e^{-M\mathbf{x}^2/2s(1-s)} \times \int_0^1 dt\,[(1-t)t]^{-\frac{3}{2}} \int d^3y e^{-M\mathbf{y}^2/2t(1-t)} \int d^3x_1'' \frac{1}{|\mathbf{x}_1''|^4}. \tag{53}$$

The variables $\mathbf{x}$ and $\mathbf{y}$ have been rescaled with respect to the original ones in order to extract the behavior of N_1 in L_1 and L_2. As a consequence, the lattices where $\mathbf{x}$ and $\mathbf{y}$ are defined have now spacings $\xi/\sqrt{L_1}$ and $\xi/\sqrt{L_2}$ respectively.

The $\mathbf{x}, \mathbf{y}$ integrals may be explicitly computed in the physical limit $L_1, L_2 >> \xi$, in which the above spacings become small. Moreover, it is possible to approximate the integral in $\mathbf{x}_1''$ with an integral over a continuous variable ρ and a cutoff in the ultraviolet region:

$$\int d^3x_1'' \frac{1}{|\mathbf{x}_1''|^4} \sim 4\pi^2 \int_\xi^\infty \frac{d\rho}{\rho^2}. \tag{54}$$

After these approximations, we finally obtain

$$N_1 = \frac{V\pi^{1/2}}{8}\frac{M^{-1}}{(8\pi)^3}(L_1L_2)^{-1/2}\xi^{-1}. \tag{55}$$

VI. CALCULATION OF SECOND AN THIRD FEYNMAN DIAGRAMS IN FIG. 2

Here we have to calculate

$$N_2 = \kappa^2 \lim_{\substack{n_1\to 0\\ n_2\to 0}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} e^{(z_1L_1+z_2L_2)} \times \int d^3x_1 d^3x_2 \int d^3x_1' d^3x_1'' d^3x_2' \times \Big\langle |\psi_1^{a_1}(\mathbf{x}_1)|^2 |\psi_2^{a_2}(\mathbf{x}_2)|^2 \left(\mathbf{A}_1\cdot\Psi_1^*\boldsymbol{\nabla}\Psi_1\right)_{\mathbf{x}_1'} \times \left(\mathbf{A}_1\cdot\Psi_1^*\boldsymbol{\nabla}\Psi_1\right)_{\mathbf{x}_1''} \left(\mathbf{A}_2^2\,|\Psi_2|^2\right)_{\mathbf{x}_2'} \Big\rangle \tag{56}$$

The above amplitude has no ultraviolet divergence, so that no regularization is required. The Wick contractions pictured in the second Feynman diagrams of Fig. 2 lead to the integral

$$N_2 = -2VL_2^{-1/2}L_1^{-1}\frac{M}{(2\pi)^6}\int_0^1 dt \int_0^t dt' C(t,t') \tag{57}$$

where $C(t,t')$ is a function independent of L_1 and L_2:

$$C(t,t') = [(1-t)t'(t-t')]^{-3/2} \times \int d^3x d^3y d^3z e^{-M(\mathbf{y}-\mathbf{x})^2/2(1-t)} \times \left(\nabla_{\mathbf{y}}^{\nu} e^{-M\mathbf{y}^2/2t'}\right)\left(\nabla_{\mathbf{x}}^{\mu} e^{-M\mathbf{x}^2/2(t-t')}\right) \times \frac{\left[\delta_{\mu\nu}\mathbf{z}\cdot(\mathbf{z}+\mathbf{x}) - (z+x)_\mu z_\nu\right]}{|\mathbf{z}|^3|\mathbf{z}+\mathbf{x}|^3}. \tag{58}$$

As in the previous section, the variables $\mathbf{x}, \mathbf{y}, \mathbf{z}$ have been rescaled with respect to the original ones in order to extract the behavior in L_1.

If the polymer lengths are much larger than the persistence length one can ignore the fact that the monomers have a finite size and it is possible to compute $C(t,t')$ analytically, leading to

$$N_2 = -\frac{V L_2^{-1/2} L_1^{-1}}{4^3 (2\pi)^6} M^{-1/2} \sqrt{2} K, \tag{59}$$

where K is the constant

$$K \equiv \frac{1}{6} B\left(\frac{3}{2}, \frac{1}{2}\right) + \frac{1}{2} B\left(\frac{5}{2}, \frac{1}{2}\right) \\ - B\left(\frac{7}{2}, \frac{1}{2}\right) + \frac{1}{3} B\left(\frac{9}{2}, \frac{1}{2}\right) = \frac{19\pi}{384} \approx 0.154, \tag{60}$$

and $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ is the Beta function. For large $L_1 \to \infty$, this diagram gives a negligible contribution with respect to N_1.

The third diagram in Fig. 2 give the same as the second, except that L_1 and L_2 are interchanged.

$$N_3 = N_2|_{L_1 \leftrightarrow L_2}. \tag{61}$$

VII. CALCULATION OF FOURTH FEYNMAN DIAGRAM IN FIG. 2

Here we have the integral

$$N_4 = -4\kappa^2 \frac{1}{2} \lim_{\substack{n_1 \to 0 \\ n_2 \to 0}} \int_{c-i\infty}^{c+i\infty} \frac{dz_1}{2\pi i} \frac{dz_2}{2\pi i} e^{(z_1 L_1 + z_2 L_2)} \\ \times \int d^3x_1 d^3x_2 \int d^3x_1' d^3x_2' d^3x_1'' d^3x_2'' \tag{62} \\ \times \Big\langle |\psi_1^{a_1}(\mathbf{x}_1)|^2 |\psi_2(\mathbf{x}_2^{a_2})|^2 (\mathbf{A}_1 \cdot \Psi_1^* \boldsymbol{\nabla} \Psi_1)_{\mathbf{x}_1'} (\mathbf{A}_1 \cdot \Psi_1^* \boldsymbol{\nabla} \Psi_1)_{\mathbf{x}_1''} \\ \times (\mathbf{A}_2 \cdot \Psi_2^* \boldsymbol{\nabla} \Psi_2)_{\mathbf{x}_2'} (\mathbf{A}_2 \cdot \Psi_2^* \boldsymbol{\nabla} \Psi_2)_{\mathbf{x}_2''} \Big\rangle.$$

which has no ultraviolet divergence. After some effort we find

$$N_4 = -\frac{1}{2 \cdot 4^6} \frac{M^3 V}{(2\pi)^{11}} (L_1 L_2)^{-1/2} \\ \times \int_0^1 ds \int_0^s ds' \int_0^1 dt \int_0^t dt' C(s,s',t,t'), \tag{63}$$

where

$$C(s,s';t,t') = [(1-s)s'(s-s')]^{-3/2} [(1-t)t'(t-t')]^{-3/2} \\ \times \int \frac{d^3p}{(2\pi)^3} \left[\epsilon_{\mu\lambda\alpha} \frac{p^\alpha}{\mathbf{p}^2} \epsilon_{\nu\rho\beta} \frac{p^\beta}{\mathbf{p}^2} + \epsilon_{\mu\rho\alpha} \frac{p^\alpha}{\mathbf{p}^2} \epsilon_{\nu\lambda\beta} \frac{p^\beta}{\mathbf{p}^2} \right] \\ \times \left[\int d^3x' d^3y' e^{-i\sqrt{L_1}\mathbf{p}(\mathbf{x}'-\mathbf{y}')} e^{-M\mathbf{x}'^2/2(1-s)} \right. \\ \times \left. \left(\nabla^\nu_{\mathbf{y}'} e^{-M\mathbf{y}'^2/2t'} \right) \left(\nabla^\mu_{\mathbf{x}'} e^{-M(\mathbf{x}-\mathbf{y})^2/2(s-s')} \right) \right] \\ \times \left[\int d^3u' d^3v' e^{-i\sqrt{L_2}\mathbf{p}(\mathbf{u}'-\mathbf{v}')} e^{-M\mathbf{v}'^2/2(1-t)} \right. \\ \times \left. \left(\nabla^\rho_{\mathbf{u}'} e^{-M\mathbf{u}'^2/2t'} \right) \left(\nabla^\lambda_{\mathbf{v}'} e^{-M(\mathbf{u}'-\mathbf{v}')^2/2(t-t')} \right) \right] \tag{64}$$

and $\mathbf{x}', \mathbf{y}'$ are scaled variables. To take into account the finite persitence length, they should be defined on a lattice with spacing $\xi/\sqrt{L_1}$. Similarly, $\mathbf{u}', \mathbf{v}'$ should be considered on a lattice with spacing $\xi/\sqrt{L_2}$. Without performing the space integrations $d^3\mathbf{x}' d^3\mathbf{y}' d^3\mathbf{u}' d^3\mathbf{v}'$, the behavior of N_4 as a function of the polymer lengths can be easily estimated in the following limits:

1. $L_1 \gg 1; L_1 \gg L_2$

$$N_4 \propto L_1^{-1} \tag{65}$$

2. $L_2 \gg 1; L_2 \gg L_1$

$$N_4 \propto L_2^{-1} \tag{66}$$

3. $L_1, L_2 \gg 1, \quad L_2/L_1 = \alpha = \text{finite}$

$$N_4 \propto L_1^{-3/2} \tag{67}$$

Moreover, if the lengths of the polymers are considerably larger than the persistence length, the function $C(s,s',t,t')$ can be computed in a closed form:

$$N_4 \approx -\frac{1}{(2\pi)^5} \frac{1}{(2\pi)^{3/2}} \frac{32}{\sqrt{2}} (L_1 L_2)^{-1/2} M^{-1/2} V \\ \times \int_0^1 ds \int_0^1 dt (1-s)(1-t)(st)^{1/2} \\ \times [L_1 t(1-s) + L_2(1-t)s]^{-1/2}. \tag{68}$$

It is simple to check that this expression has exactly the above behaviors.

VIII. FINAL RESULT

Collecting all contributions we obtain the result for the second topological moment:

$$\langle m^2 \rangle = \frac{N_1 + N_2 + N_3 + N_4}{Z}, \tag{69}$$

with N_1, N_2, N_3, N_4, Z given by Eqs. (36), (55), (59), (61), and (68).

In all formulas, we have assumed that the volume V of the system is much larger than the size of the volume occupied by a single polymer, i.e., $V \gg L_1^3$

To discuss the physical content of the result (69), we assume P_2 to be a long effective polymer representing all polymers in a uniform solution. We introduce the polymer concentration ρ as the average mass density of the polymers per unit volume:

$$\rho = \frac{M}{V} \tag{70}$$

where M is the total mass of the polymers

$$M = \sum_{i=1}^{N_p} m_a \frac{L_k}{a}. \tag{71}$$

Here m_a is the mass of a single monomer of length a, L_k is the length of polymer P_k, and N_p is the total number of polymers. Thus L_k/a is the number of monomers in the polymer P_k. The polymer P_1 is singled out as any of the polymers P_k, say $P_{\bar{k}}$, of length $L_1 = L_{\bar{k}}$. The remaining ones are replaced by a long effective polymer P_2 of length $L_2 = \sigma_{k \neq \bar{k}} L_k$. From the above relations we may also write

$$L_2 \approx \frac{aV\rho}{m_a} \tag{72}$$

In this way, the length of the effective molecule P_2 is expressed in terms of physical parameters, the concentration of polymers, the monomer length, and the mass and volume of the system. Inserting (72) into (69), with N_1, N_2, N_3, N_4, Z given by Eqs. (36), (55), (59), (61), and (68). and keeping only the leading terms for $V \gg 1$, we find for the second topological moment $\langle m^2 \rangle$ the approximation

$$\langle m^2 \rangle \approx \frac{N_1 + N_2}{Z}, \tag{73}$$

and this has the approximate form

$$\langle m^2 \rangle = \frac{a\rho}{m_a} \left[\frac{\xi^{-1} L_i}{16\pi^{1/2} M^2} - \frac{K\sqrt{2} L_1^{1/2}}{(2\pi)^4 M^{3/2}} \right], \tag{74}$$

with K of (60).

IX. SUMMARY

We have set up a topological field theory to describe two fluctuating polymers P_1 and P_2, and calculated the second topological moment for the linking number m between P_1 and P_2. The result is used to calculate the second moment for a single polymer with respect to all others in a solution of many polymers.

In forthcoming work we shall calculate the effect of the excluded volume.

X. APPENDIX

In this appendix we present the computations of the amplitudes $N_1, \ldots, N_4$. We shall need the following simple tensor formulas involving two completely antisymmetric tensors $\varepsilon^{\mu\nu\rho}$:

$$\varepsilon_{\mu\nu\rho} \varepsilon^{\mu\alpha\beta} = \delta_\nu^\alpha \delta_\rho^\beta - \delta_\nu^\beta \delta_\rho^\alpha \tag{75}$$

$$\varepsilon_{\mu\nu\rho} \varepsilon^{\mu\nu\beta} = 2\delta_\rho^\beta. \tag{76}$$

The Feynman diagrams shown in Fig. 2) corresponds to a product of four correlation functions G_0 of Eq. (39), which have to be integrated over space and Laplace transformed. For the latter we make use of the convolution property of the integral over two Laplace transforms $\tilde{f}(z)$ and $\tilde{g}(z)$ of the functions f, g:

$$\int_{c-i\infty}^{c+i\infty} \frac{dz}{2ni} e^{zL} \tilde{f}(z) \tilde{g}(z) = \int_0^L ds f(s) g(L-S) \tag{77}$$

All spatial integrals are Gaussian of the form

$$\int d^3x e^{-a\mathbf{x} + 2b\mathbf{x}\cdot\mathbf{y}} = (2n)^{3/2} a^{-3/2} e^{b^2 y^2/a}, \quad a > 0. \tag{78}$$

We are now ready to evaluate N_1 in Eq. (52). Taking the limit of vanishing replica indices we find with the help of Eqs. (75)-(77):

$$\begin{aligned} N_1 = &\int d^3x_1, d^3x_2 \int_0^{L_1} ds \int_0^{L_2} dt \int d^3x_1' d^3x_2' \\ &\times G_0(\mathbf{x}_1 - \mathbf{x}_1'; s) G_0(\mathbf{x}_1' - \mathbf{x}_1; L_1 - S) \\ &\times G_0(\mathbf{x}_2 - \mathbf{x}_2'; t) G_0(\mathbf{x}_2' - \mathbf{x}_2; L_2 - t) \frac{l}{|\mathbf{x}_1' - \mathbf{x}_2'| s}. \end{aligned} \tag{79}$$

Performing the changes of variables

$$s' = \frac{s}{L_1} \quad t' = \frac{t}{L_2} \quad \mathbf{x} = \frac{\mathbf{x}_1 \mathbf{x}_1'}{\sqrt{4}} \quad \mathbf{y} = \frac{\mathbf{x}_2 - \mathbf{x}_2'}{(\sqrt{L_2})} \tag{80}$$

and setting $\mathbf{x}_1'' \equiv \mathbf{x}_1' - \mathbf{x}_2'$, we easily derive (53).

For small $\xi/\sqrt{L_1}$ and $\xi/\sqrt{L_2}$, we d use the approximation (54), the space integrals can be done the formula (78). After some calculation one finds the final result of Eq. (66).

The amplitude N_2 calculated quite similarly. Contracting the fields in Eq. (56), and keeping only the contributions which do not vanish in the limit of zero replica indices, we arrive at

$$\begin{aligned} N_2 = &\int d^3x_1 d^3x_2 \int d^3x_1' d^3x_1'' d^3x_2' \\ &\times \left[\int_0^{L_1} ds \int_0^S ds' G_0(\mathbf{x}_1' - \mathbf{x}_1; L_1 - s) \right. \\ &\times \left. \nabla_{x_1''}^\nu G_0(\mathbf{x}_1 - \mathbf{x}_1''; s') \nabla_{x_1'}^\mu G_0(\mathbf{x}_1'' - \mathbf{x}_1'; s - s') \right] \\ &\times D_{\mu\lambda}(\mathbf{x}_1' - \mathbf{x}_2) D_{\nu\lambda}(\mathbf{x}_1'' - \mathbf{x}_2') \\ &\times \left[\int_0^{L_2} dt G_0(\mathbf{x}_2 - \mathbf{x}_2'; L_2 - t) G_0(\mathbf{x}_2' - \mathbf{x}_2; t) \right]. \end{aligned} \tag{81}$$

where $D_{\mu\nu}(\mathbf{x}, \mathbf{x}')$ are the correlation functions (9)–(10) of the vector potentials. Setting $\mathbf{x}_2 \equiv \sqrt{L_2}\mathbf{u} + \mathbf{x}_2'$ and

supposing that $\xi/\sqrt{L_2}$ is small, the integral over $\mathbf{u}$ can be easily evaluated with the help of the Gaussian integral (78). After the substitutions $\mathbf{x}_1'' = \sqrt{L_1}\mathbf{y} + \mathbf{x}_1 \quad \mathbf{x}_1' = \sqrt{L_1}(\mathbf{y} - \mathbf{x}) + \mathbf{x}_1, \quad \mathbf{x}_2' = \sqrt{L_1}(\mathbf{y} - \mathbf{x} - \mathbf{z}) + \mathbf{x}_1$ and a rescaling of the variables s, s' by a factor L_1^{-1}, we derive Eq. (57) with (58).

For small $\xi/\sqrt{L_1}$, $\frac{3}{\sqrt{L_2}}$, the spatial integrals are easily evaluated leading to:

$$N_2 = \frac{-\sqrt{2}VL_2^{-1/2}L_1^{-1}M^{-1/2}}{(4n)^6} \int_0^1 dt \int_0^t dt' t'(1-t)\sqrt{\frac{t-t'}{1-t+t'}} \tag{82}$$

After the change of variable $t' \to t'' = t - t'$, the double integral is reduced to a sum of integrals the type

$$c(n,m) = \int_0^1 dt t^m \int_0^t dt' t'^n \sqrt{\frac{t'}{1-t'}}, \quad m, n = \text{integers.}$$

These can be simplified by replacing t^m by $dt^{m+1}/dt(m+1)$, and doing the integrals by parts. In this way, we end up with a linear combination of integrals of the form:

$$\int_0^1 dt \frac{t^{\mu+\frac{1}{2}}}{\sqrt{1-t}} = B\left(\mu + \frac{3}{2}, \frac{1}{2}\right). \tag{83}$$

The calculations of N_3 and N_4 are very similar, and may be omitted here.

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